



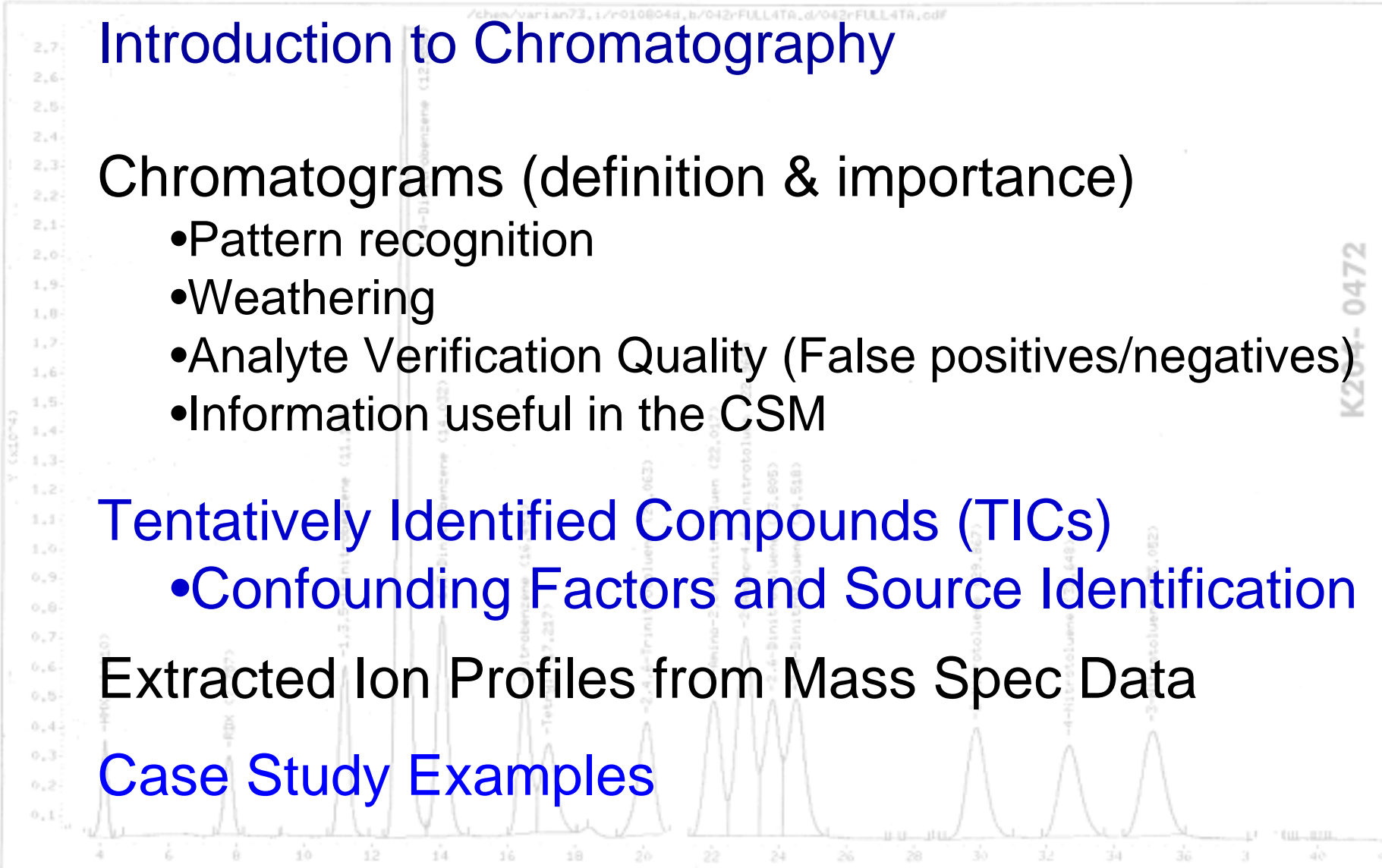
Chromatograms: The Untold Story

Ed Corl

Atlantic Division Environmental

**IR Conference
February 2004**

Case Study Examples



Data File: /chem/varian73.i/r010604d.b/042rFULL4TA.d
 Date : 05-MIG-2001 09:54
 Client ID: FULL4TA
 Sample Info: FULL4TA
 Volume Injected (uL): 25.0
 Column: 042rFULL4TA.d

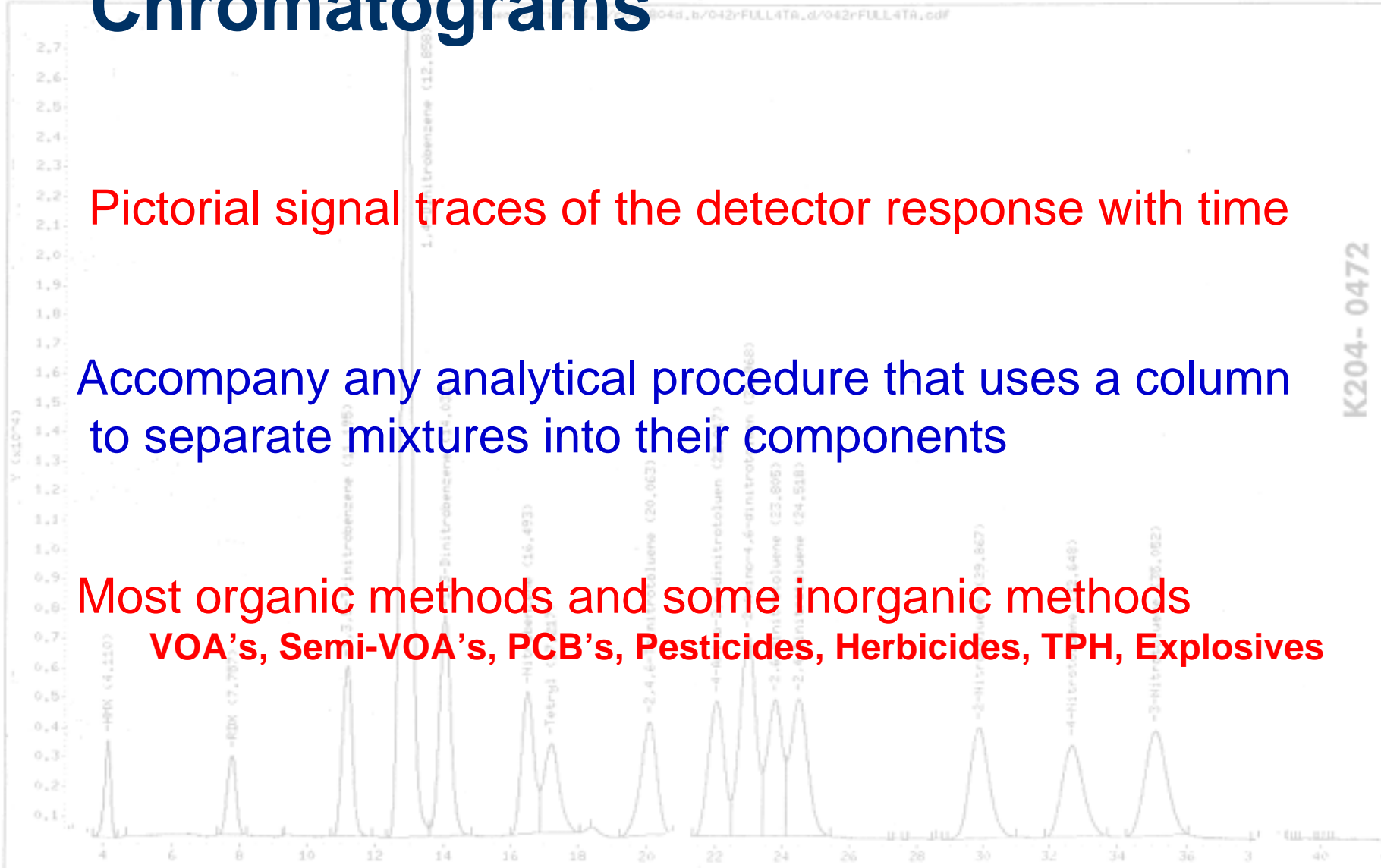
Instrument: varian73.i
 Operator: 2401
 Column diameter: 3.90

Chromatograms

Pictorial signal traces of the detector response with time

Accompany any analytical procedure that uses a column to separate mixtures into their components

Most organic methods and some inorganic methods
 VOA's, Semi-VOA's, PCB's, Pesticides, Herbicides, TPH, Explosives



K204- 0472

Data File: /chem/varian73.1/r010804d,b/042rFULL4TA,d
Date : 05-AUG-2001 09:54
Client ID: FULL4TA
Sample Info: FULL4TA
Volume Injected (uL): 25.0
Column phase: C8

Instrument: varian
Operator: 2401
Column diameter: 3.90

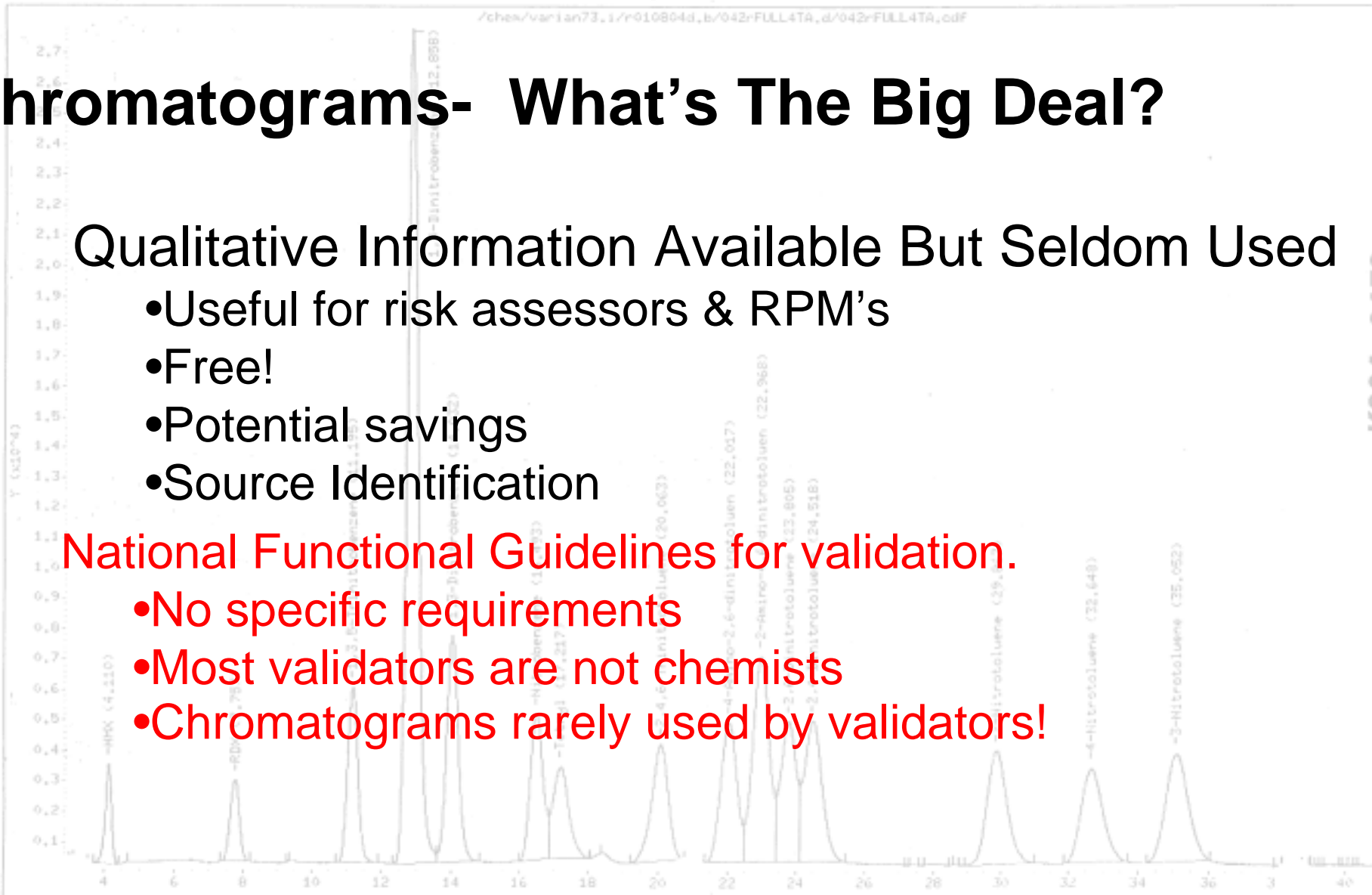
Chromatograms- What's The Big Deal?

Qualitative Information Available But Seldom Used

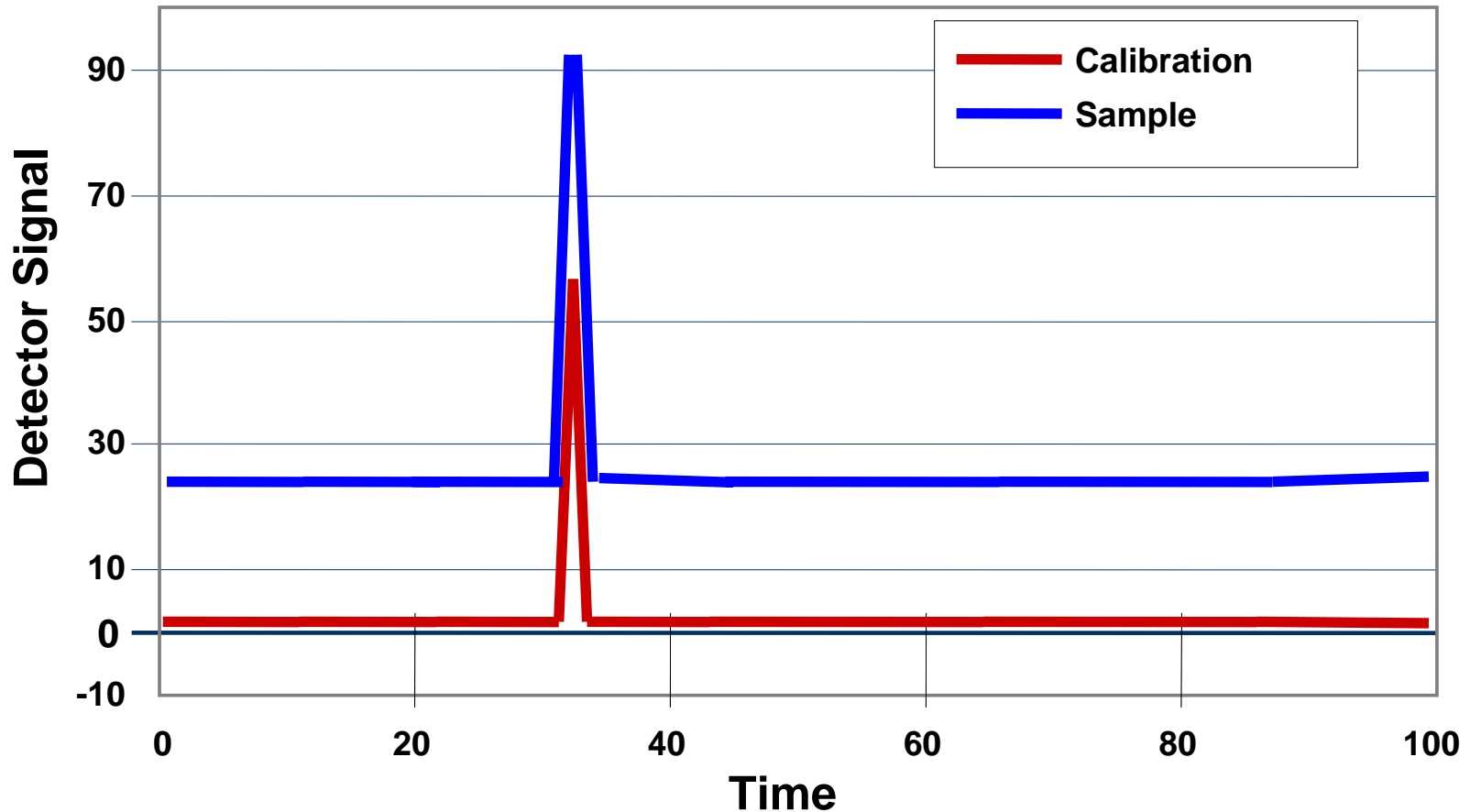
- Useful for risk assessors & RPM's
- Free!
- Potential savings
- Source Identification

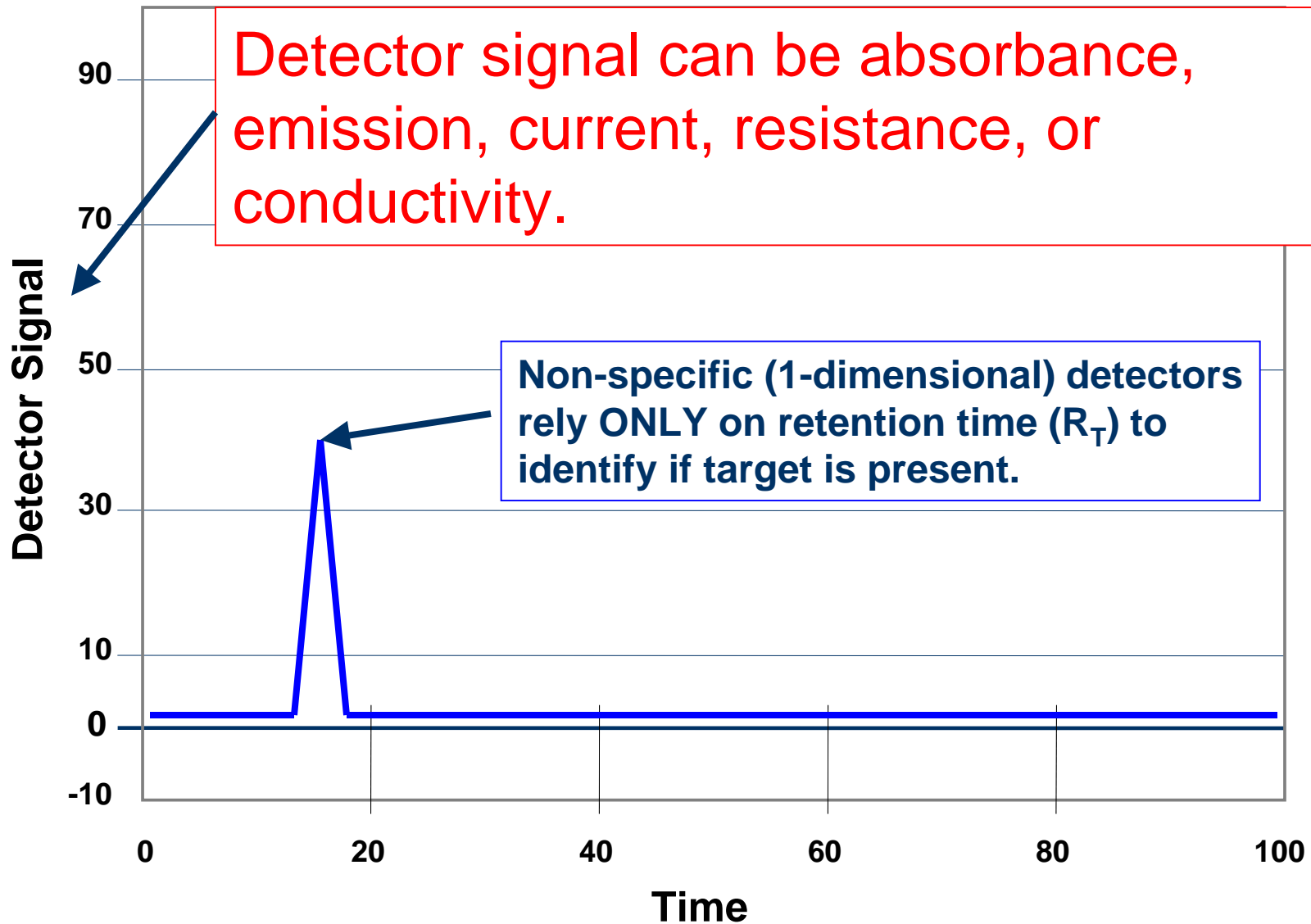
National Functional Guidelines for validation.

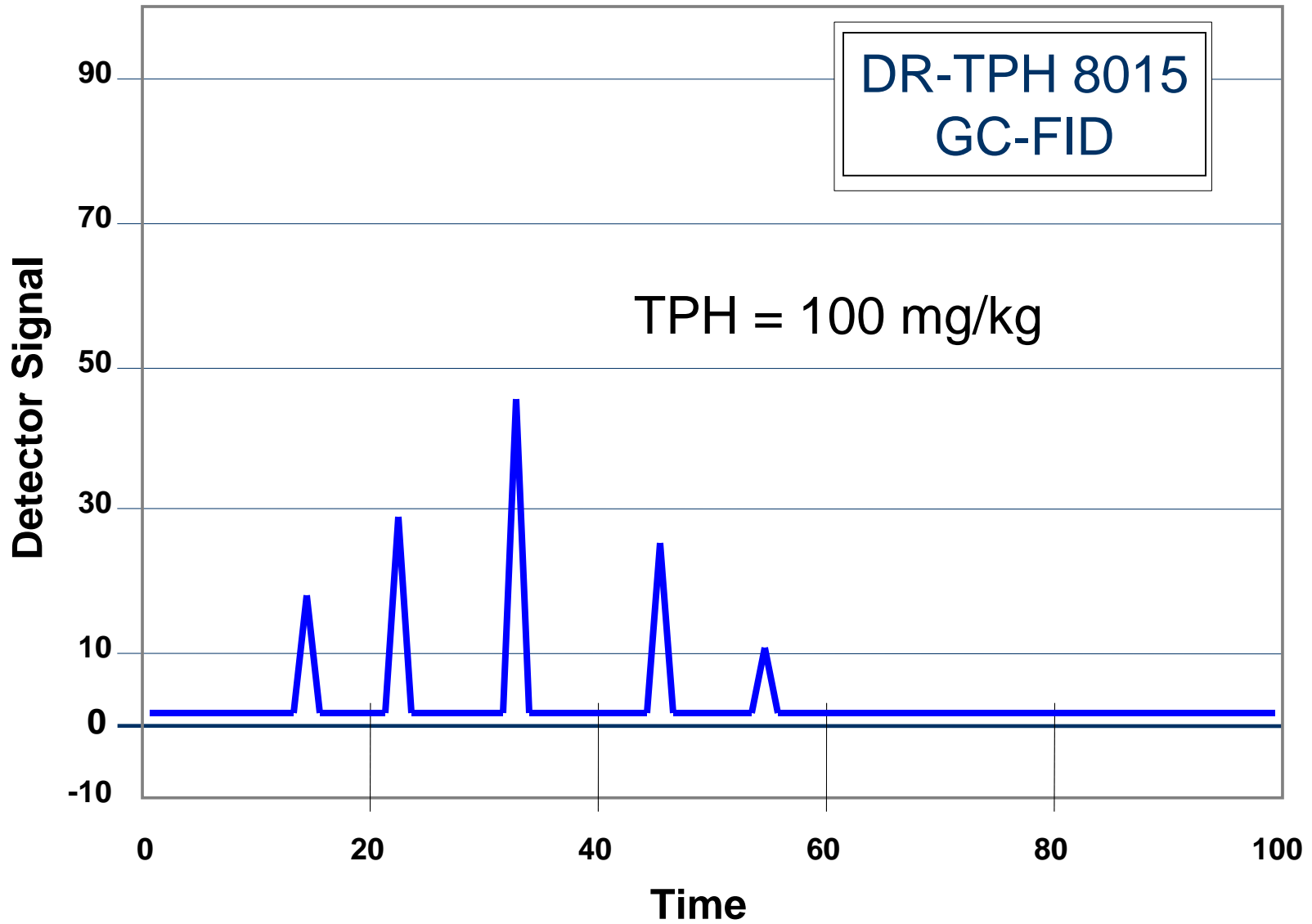
- No specific requirements
- Most validators are not chemists
- Chromatograms rarely used by validators!



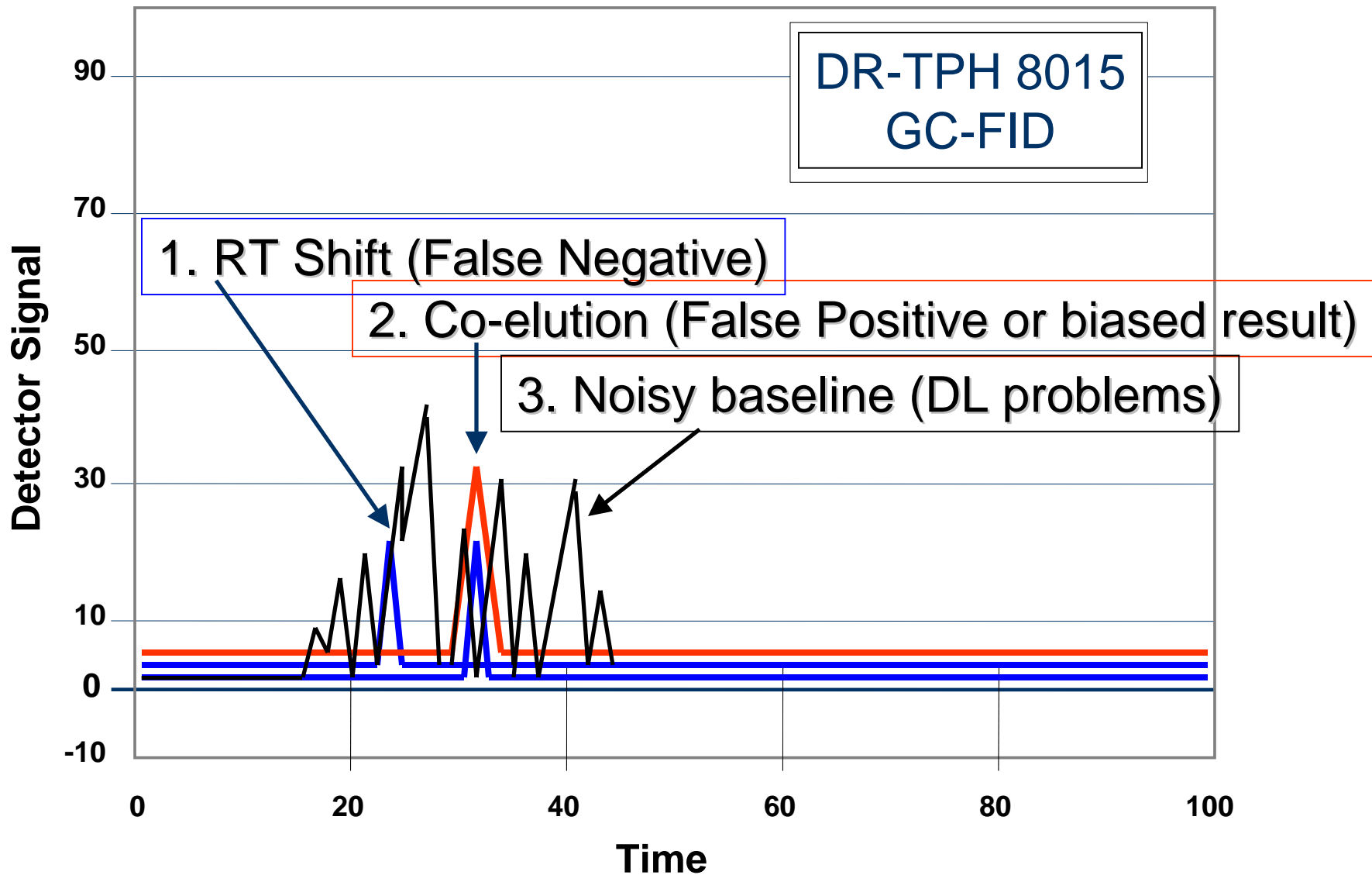
Retention time qualification







Potential Chromatographic Problems

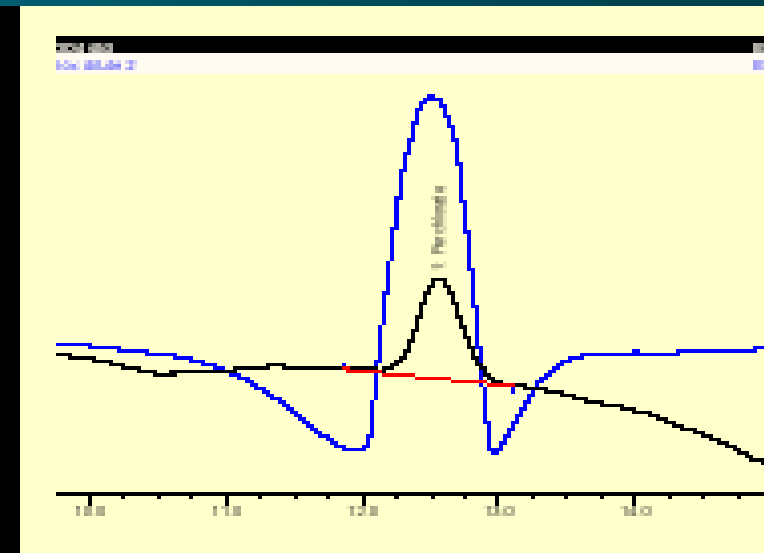


- TPH (8015)-Flame ionization (FID)
- PCB (8081/2)-Electron Capture (ECD)
- Pesticides (8081/2)- (ECD)
- Herbicides (8141)-Nitrogen/Phosphorus (NPD)
- Explosives (8330)-Diode Array UV
- Perchlorates (314/9058)-Conductivity



There are Interfering Substances -e.g. Alconox..

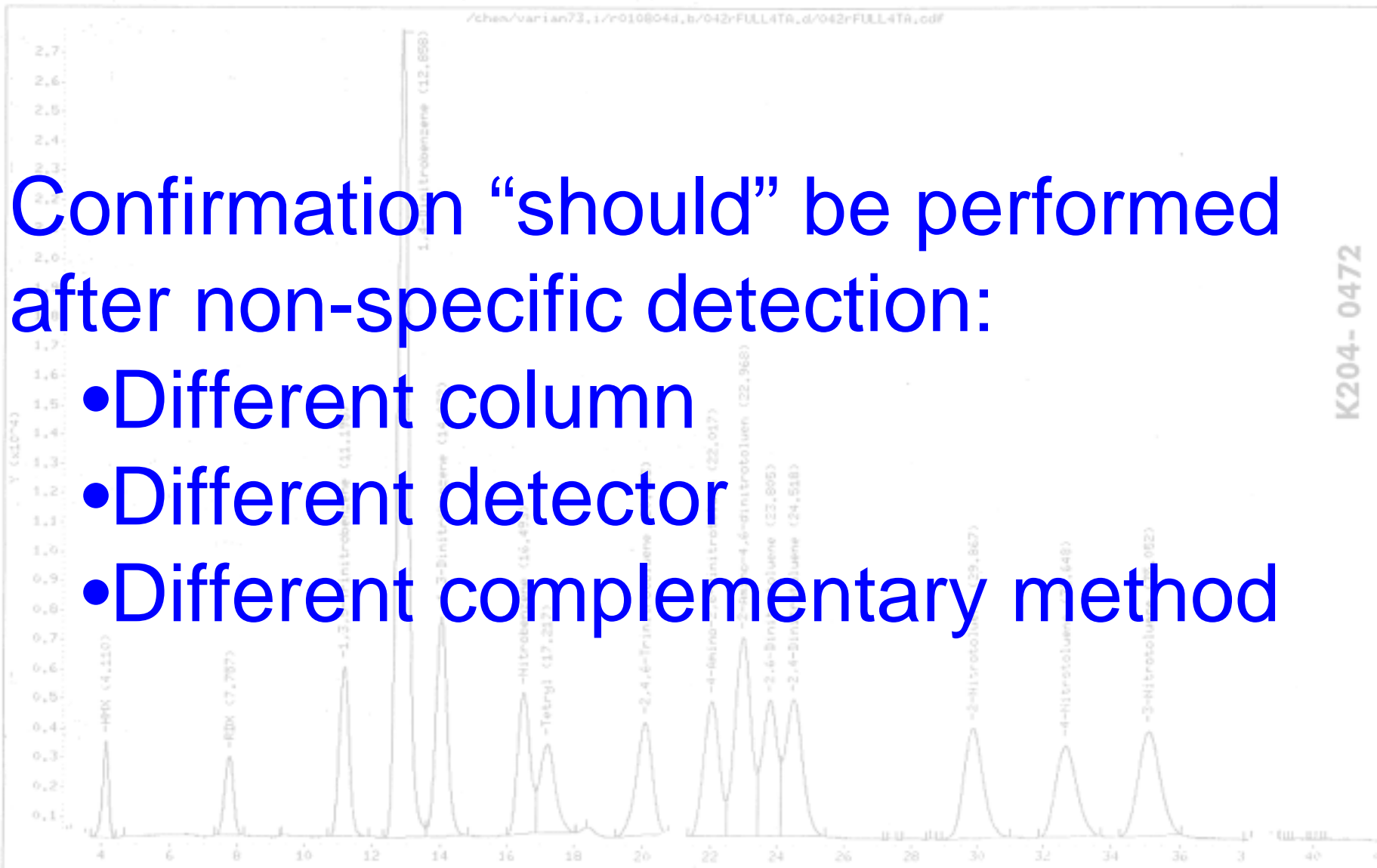
Like any analytical method, be aware of the potential for interference, but this one will be unlikely in drinking water.



Most reported chromatographic interferences are from waste sites

Data File: /chem/varian73.i/r010804d.b/042rFULL4TA.d
 Date : 05-MIG-2001 09:54
 Client ID: FULL4TA
 Sample Info: FULL4TA
 Volume Injected (uL): 25.0
 Column phase: CB

Instrument: varian73.i
 Operator: 2401
 Column diameter: 3.90



Confirmation “should” be performed after non-specific detection:

- Different column
- Different detector
- Different complementary method

Column diameter: 3,90

04d,b/042rFULL4TA,d/042rFULL4TA,d#

- GRO or DRO by method 8015 (GC-FID)

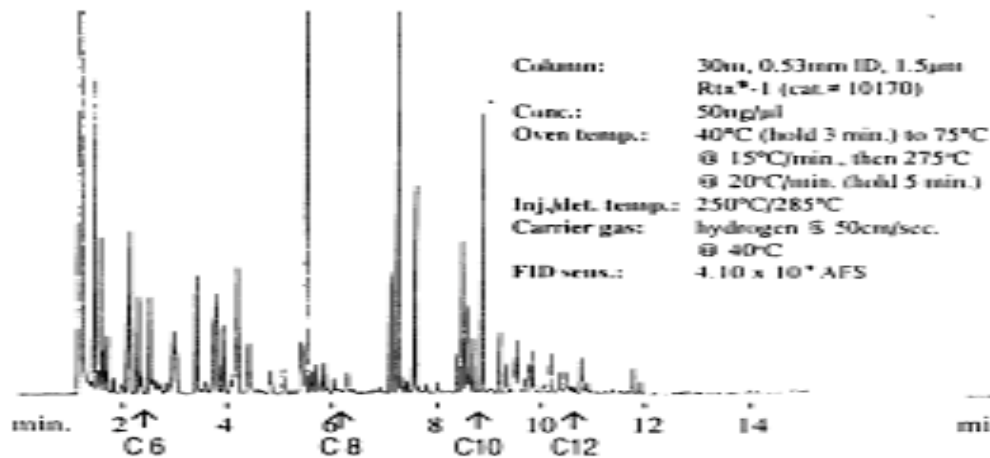
- Prone to false positives

- Weathering
- Integration errors/confirmation
- Type of TPH fingerprint

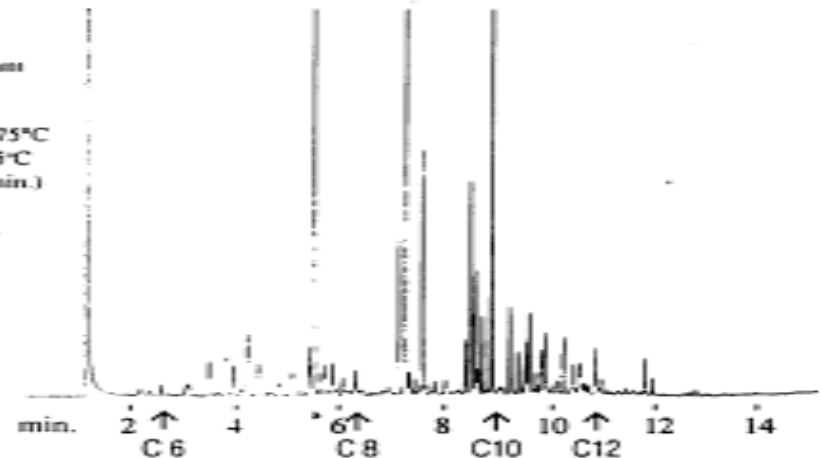


TPH-Qualitative Data (weathering)

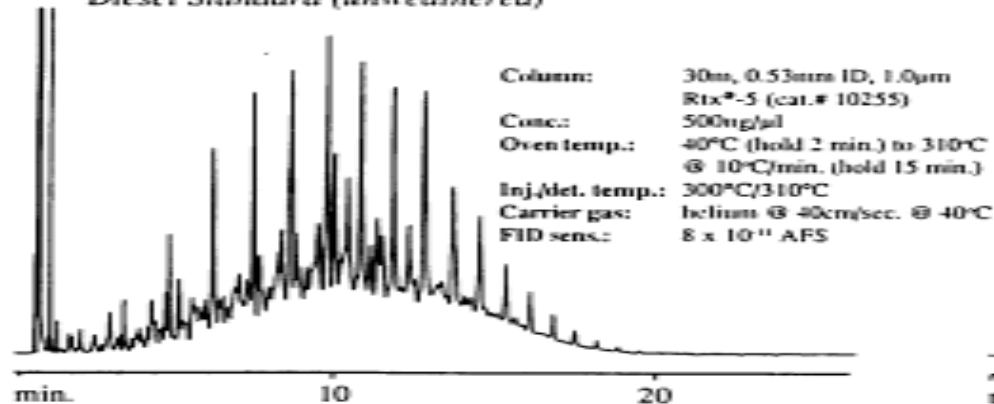
Unleaded Gasoline Standard (unweathered)



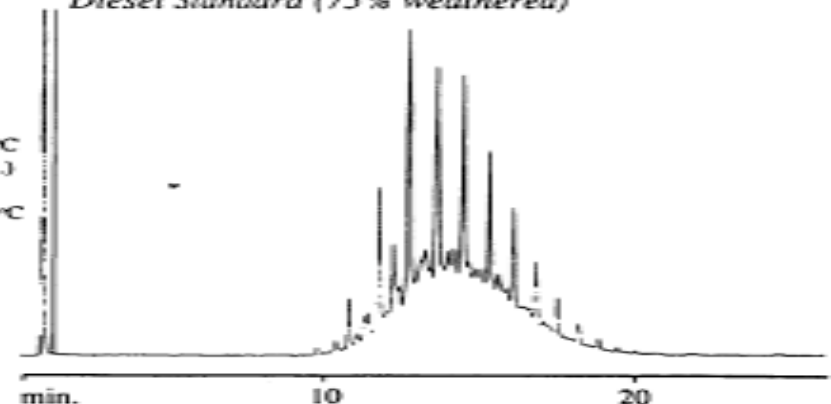
Unleaded Gasoline (50% weathered)



Diesel Standard (unweathered)

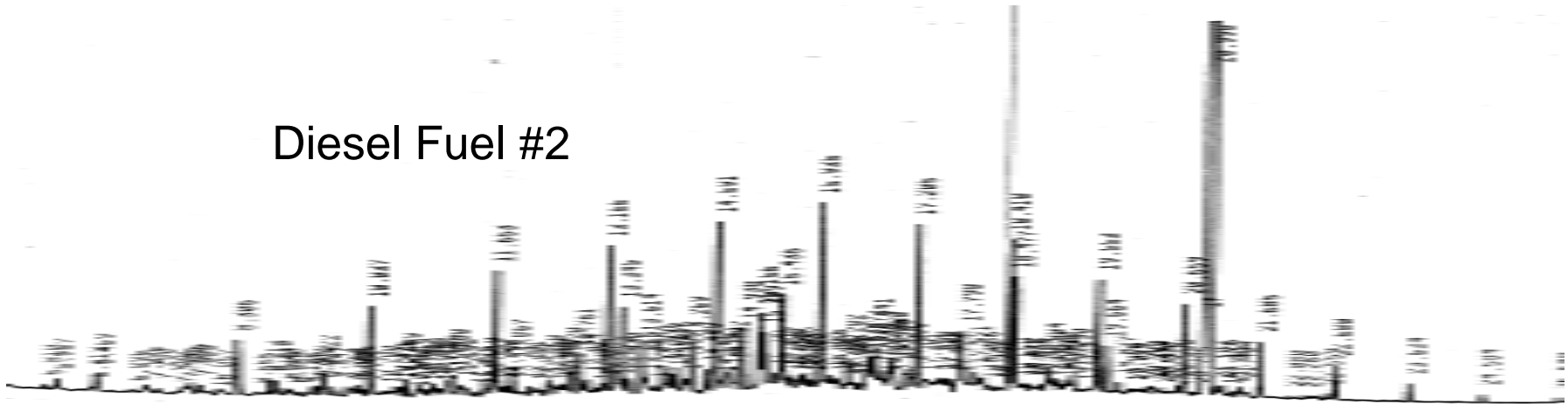


Diesel Standard (75% weathered)

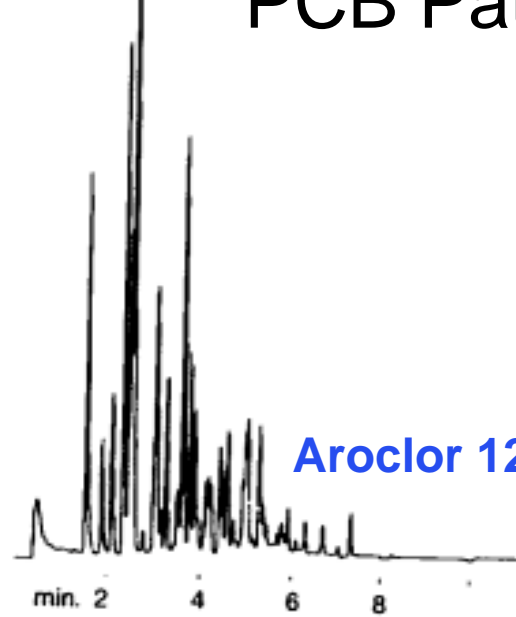


TPH- Pattern Recognition

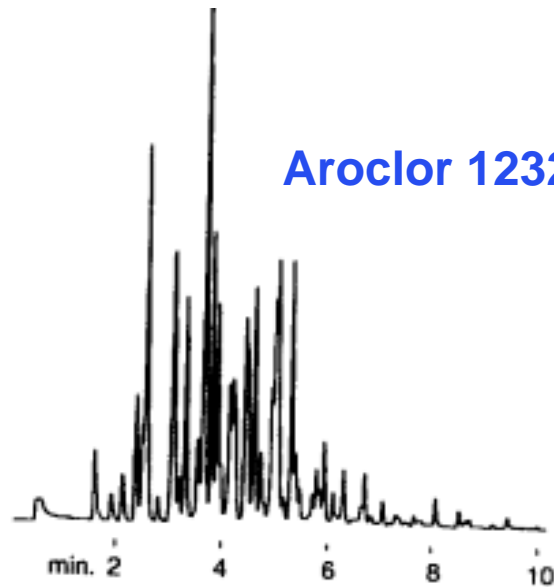
Diesel Fuel #2



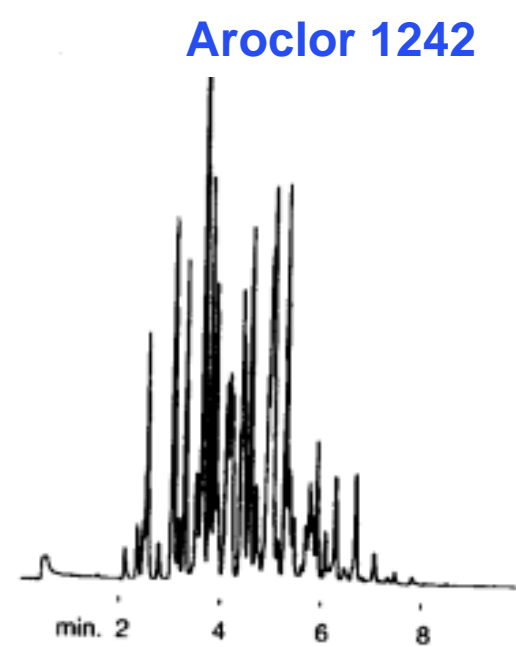
PCB Pattern Recognition



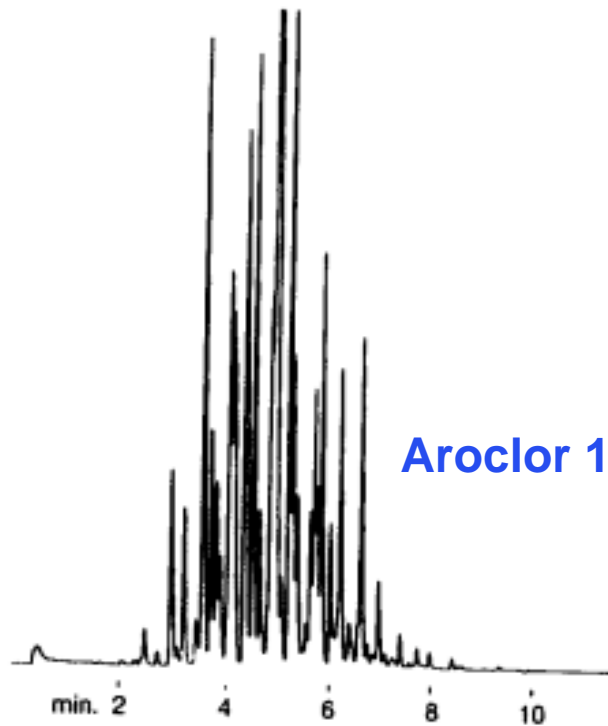
Aroclor 1221



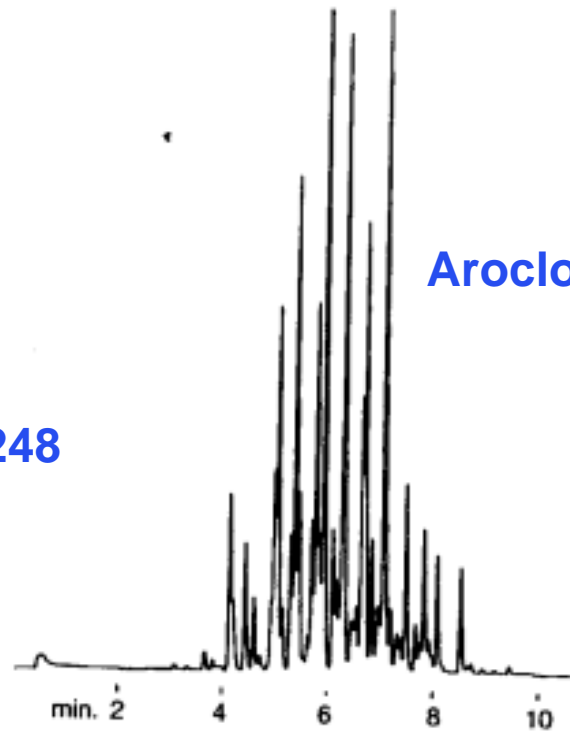
Aroclor 1232



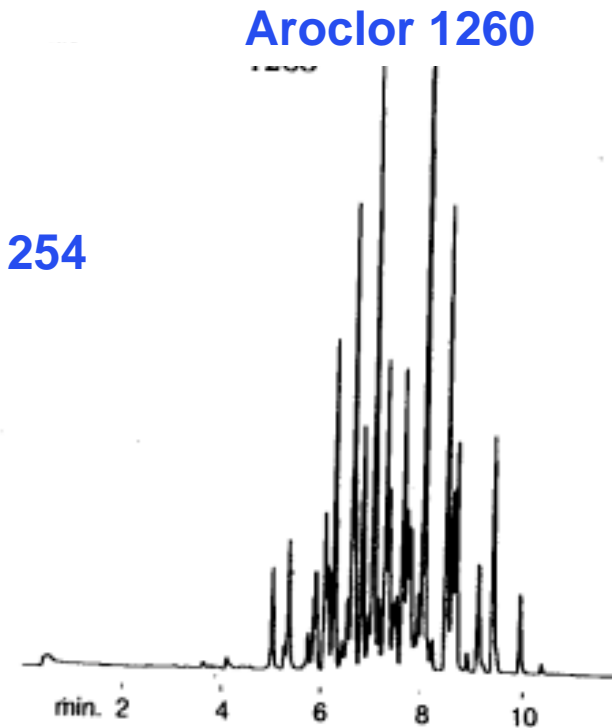
Aroclor 1242



Aroclor 1248

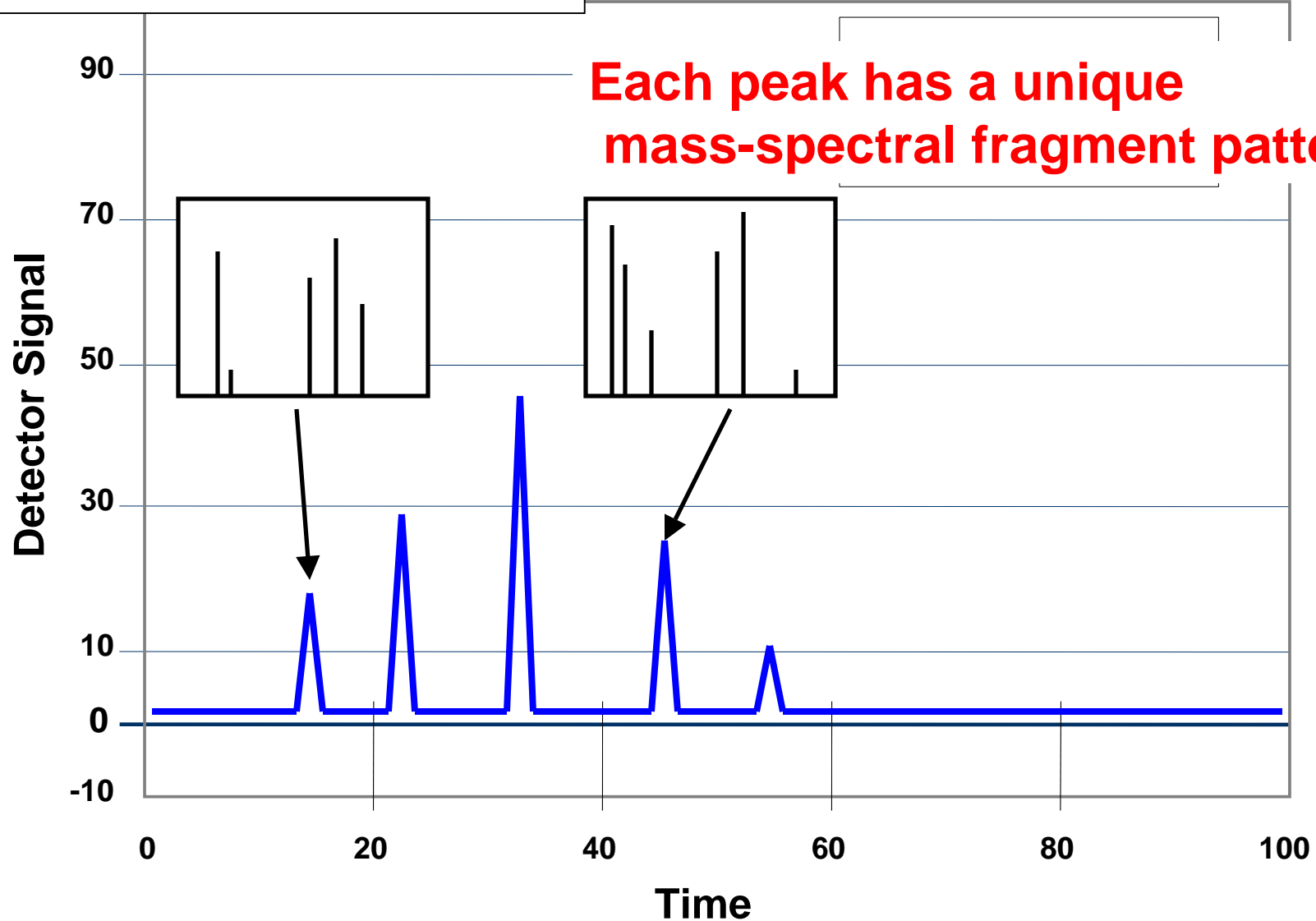


Aroclor 1254



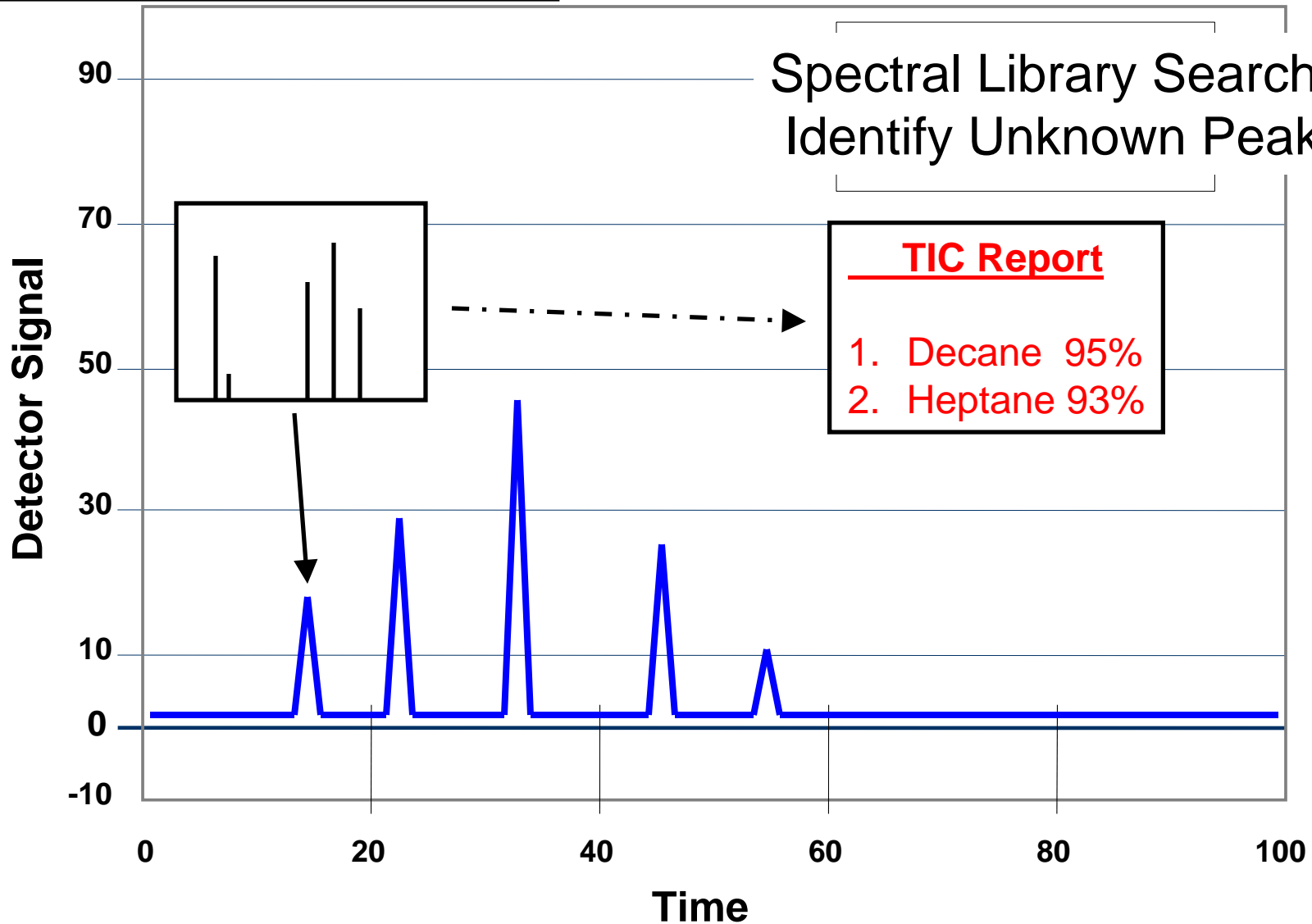
Aroclor 1260

Mass Spectrometry 2-Dimensional Detector

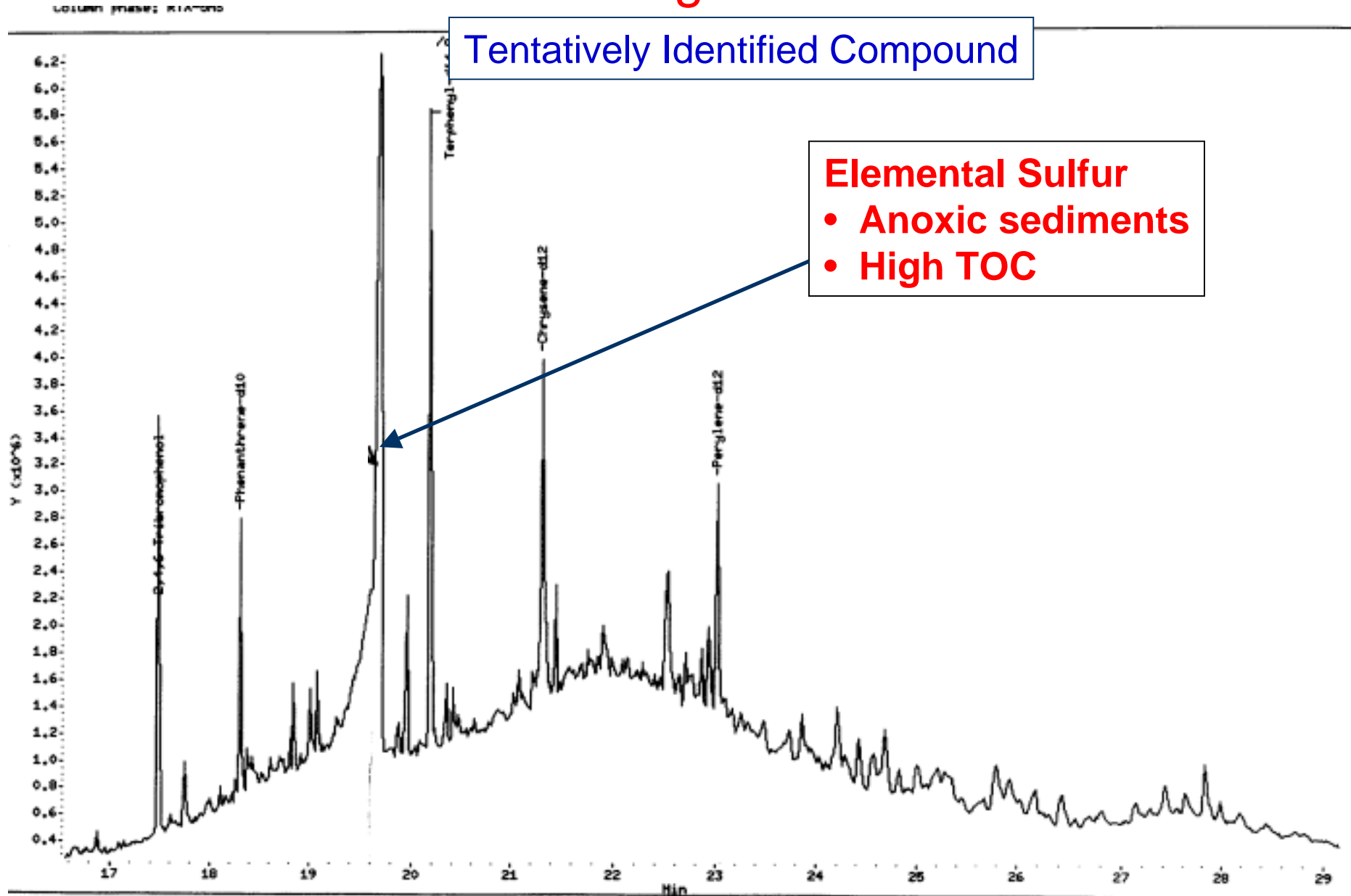


Tentatively Identified Compounds (TIC)

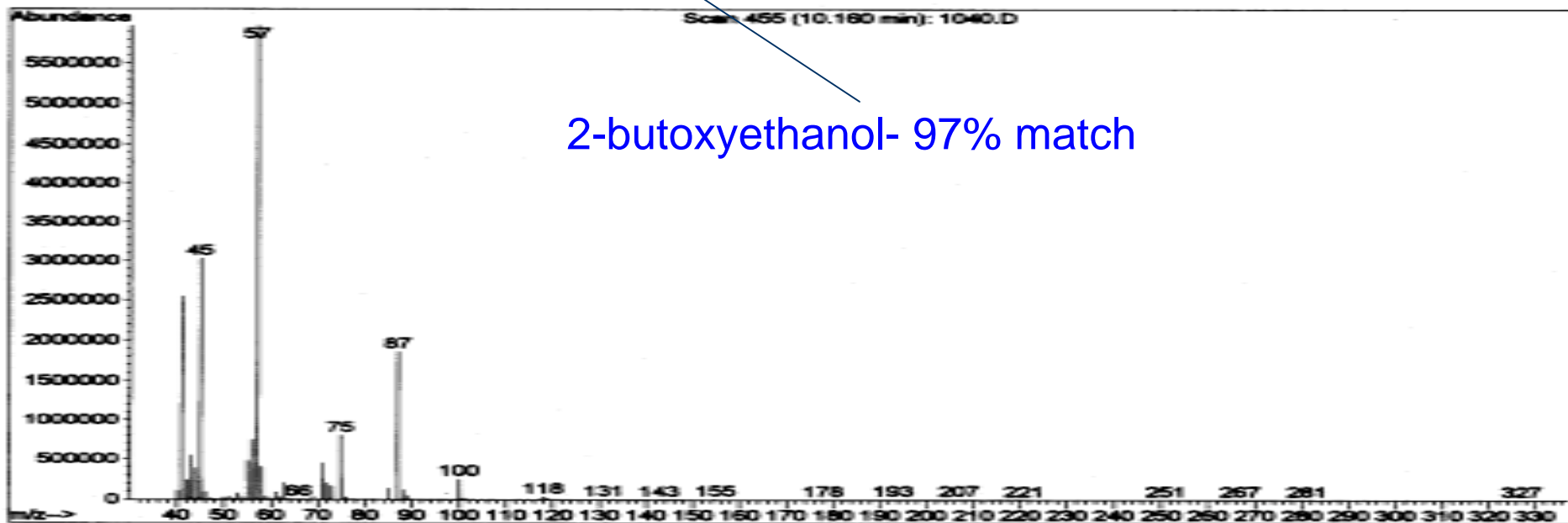
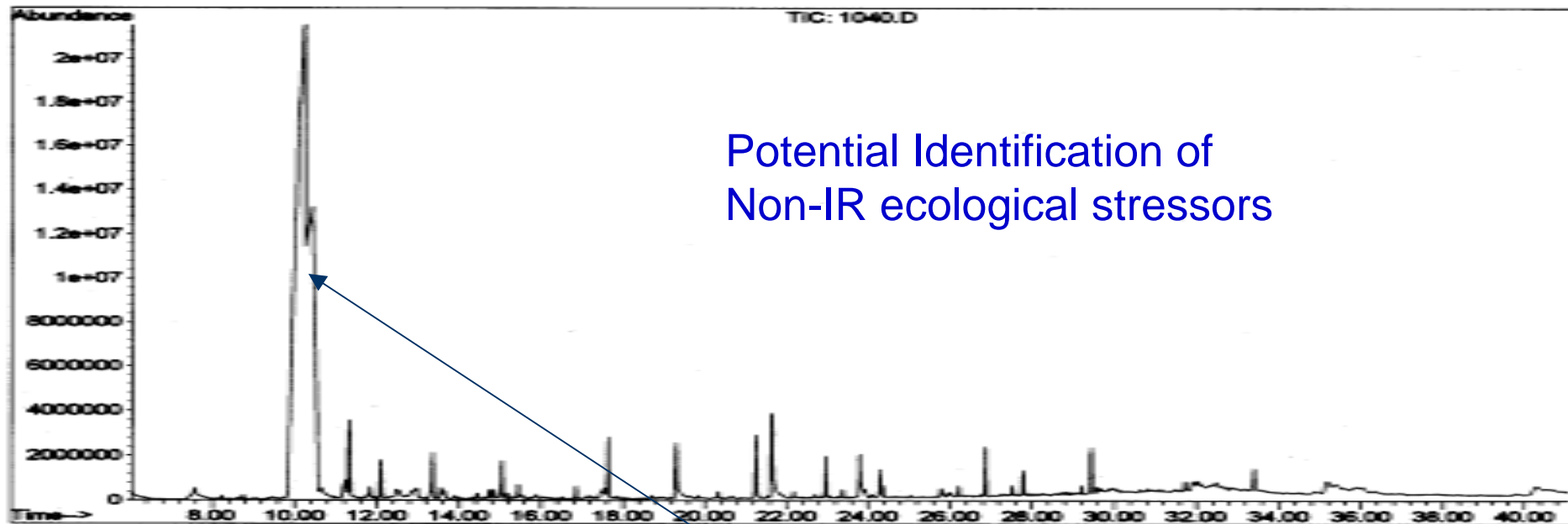
Spectral Library Search to
Identify Unknown Peaks



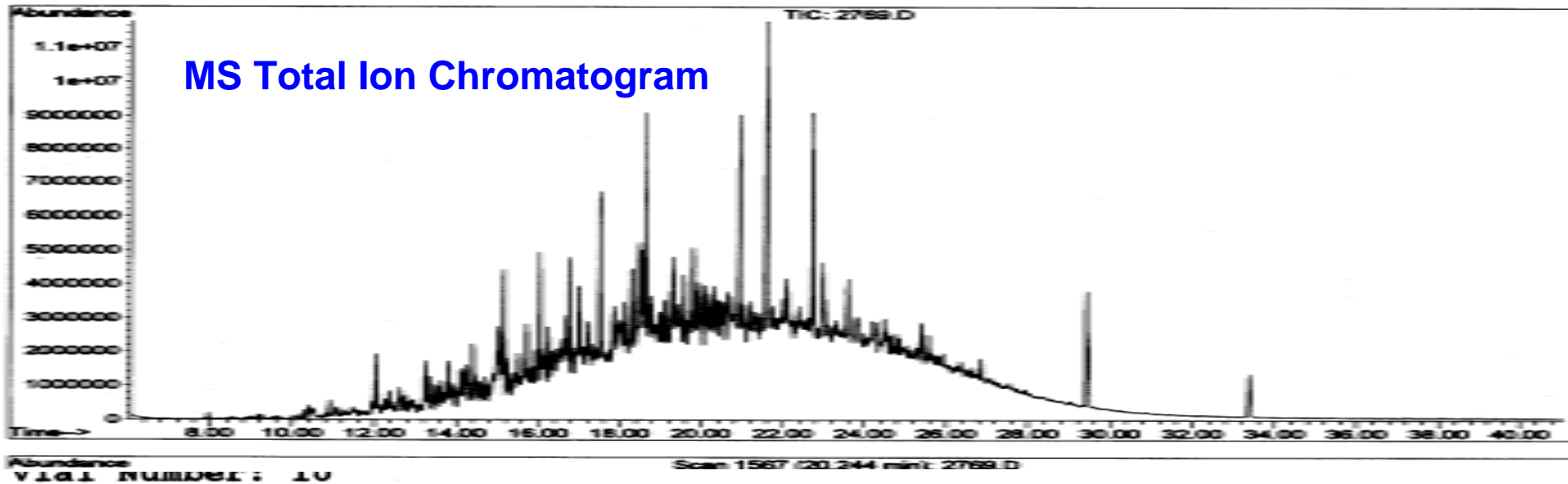
GC/MS Chromatogram Review



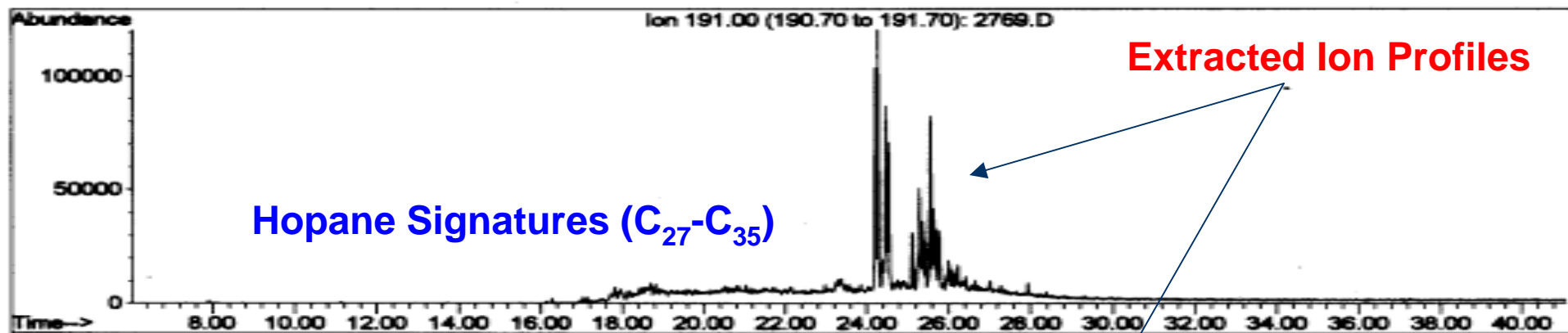
Tentatively Identified Compounds (TICs)



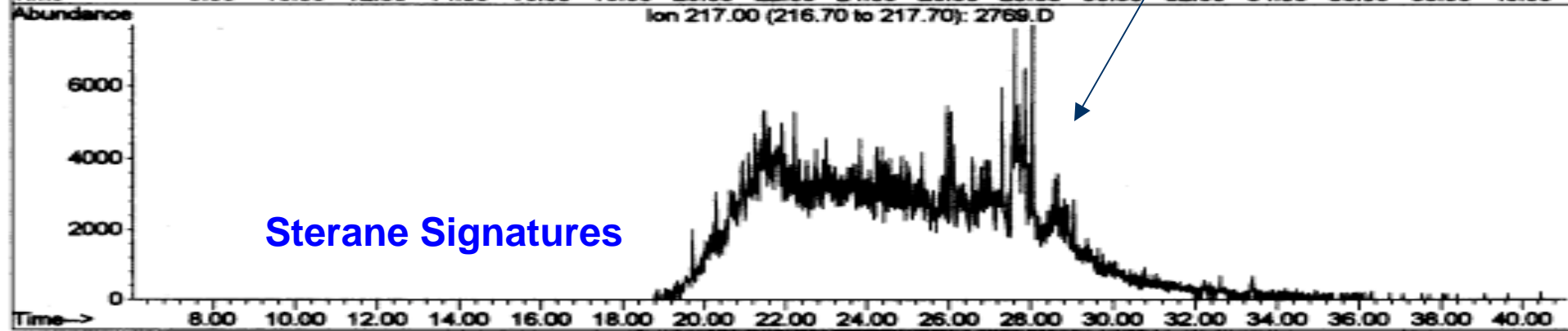
MS Total Ion Chromatogram



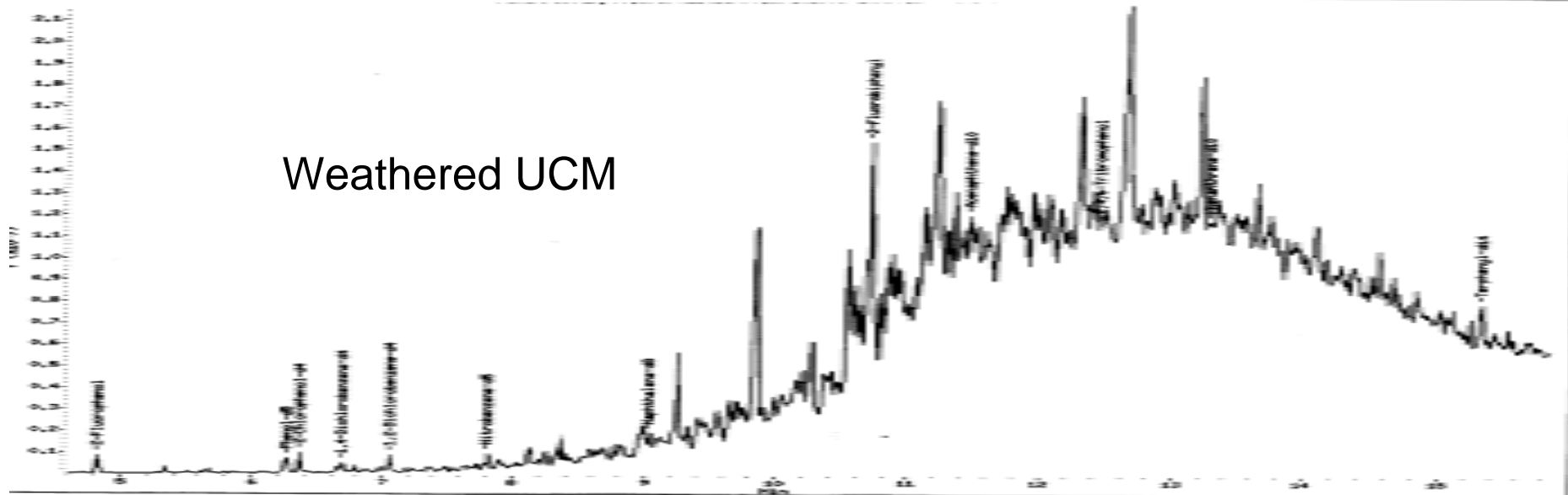
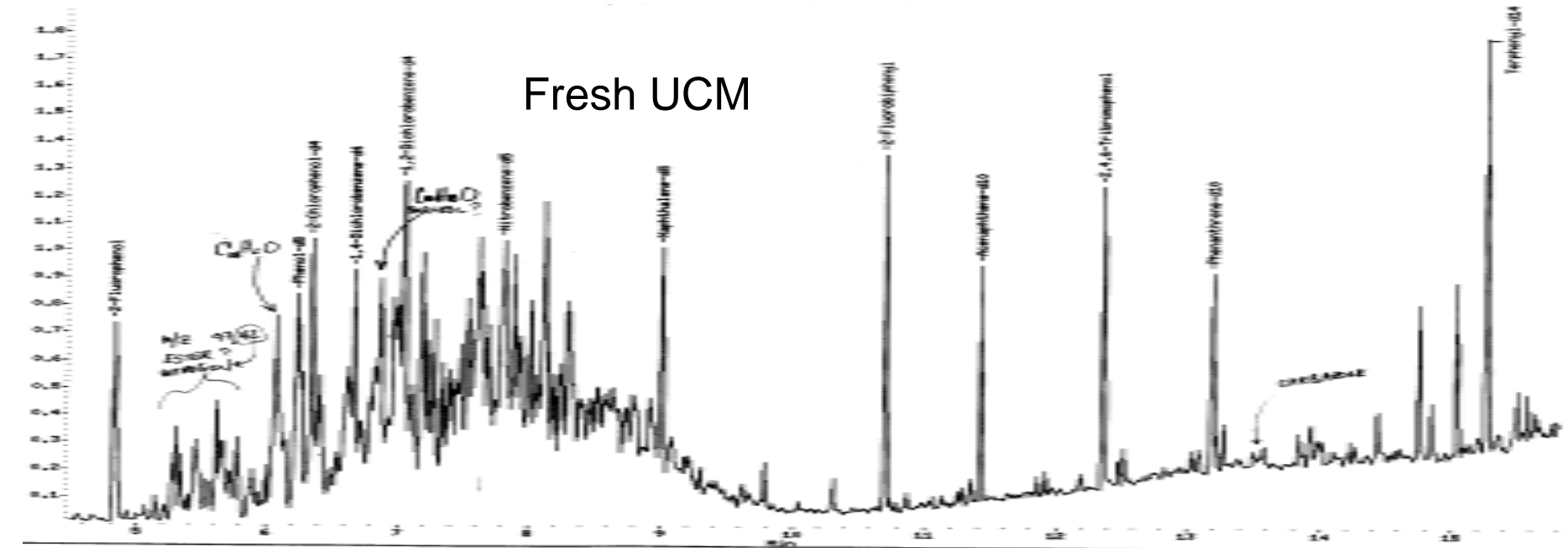
Hopane Signatures (C_{27} - C_{35})



Sterane Signatures



CSM Information- Identification of Current sources



/chem/varian73,i/r010@04d,b/042rFULL4TA,d/042rFULL4TA.cd#

- Chromatograms give vital qualitative information
- Important data quality information
- Fingerprints can be used by non-chemists
- Free but seldom utilized
- Mass Spec/Tentatively Identified Compounds
- Existing MS Datafiles can be used for potential Identification via Fingerprints and Ion Profiles



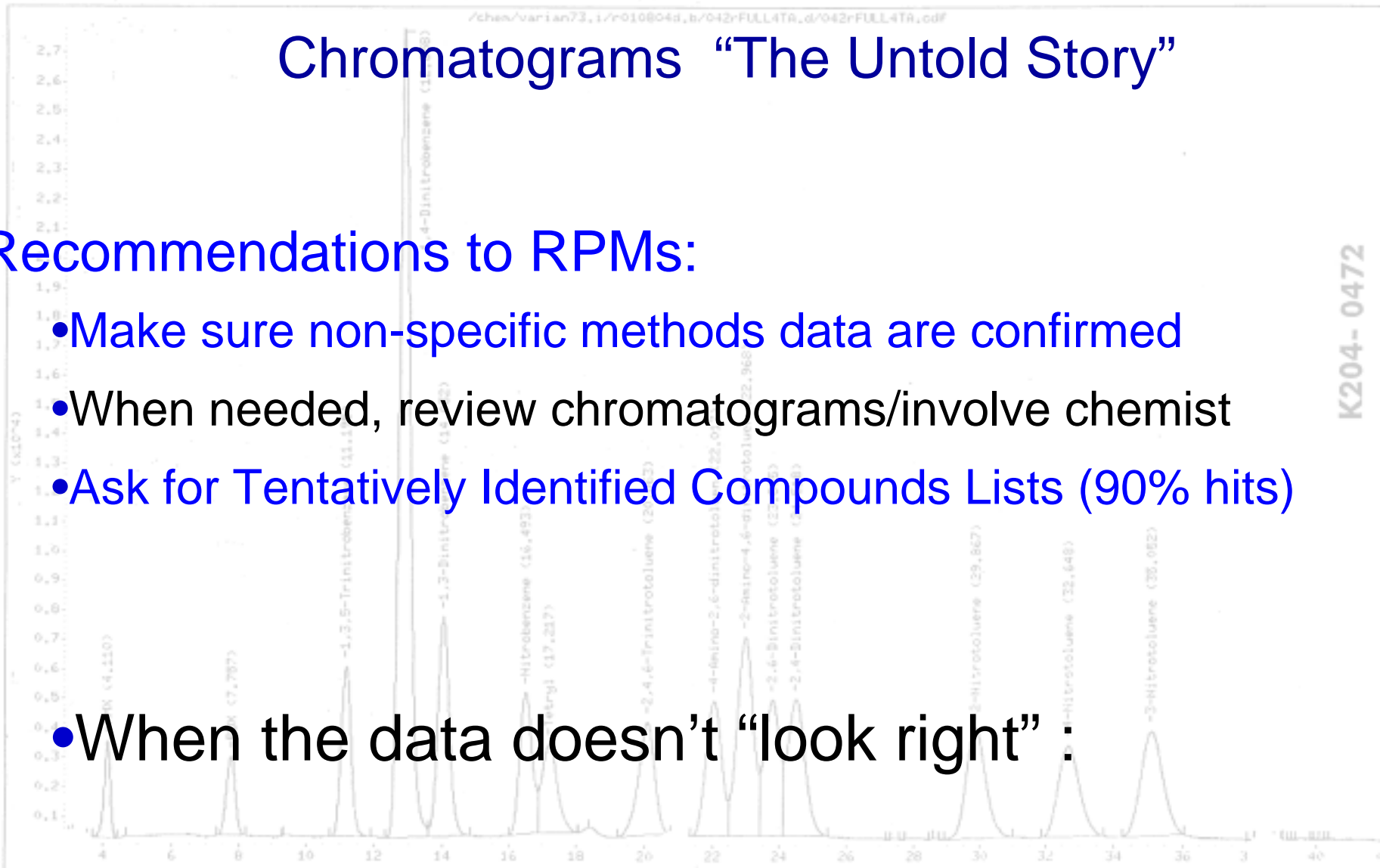
Data File: /chem/varian73.i/r010804d.b/042rFULL4TA.d
 Date : 05-MIG-2001 09:54
 Client ID: FULL4TA
 Sample Info: FULL4TA
 Volume Injected (uL): 25.0
 Column phase: CB

Instrument: varian73.i
 Operator: 2401
 Column diameter: 3.90

Chromatograms “The Untold Story”

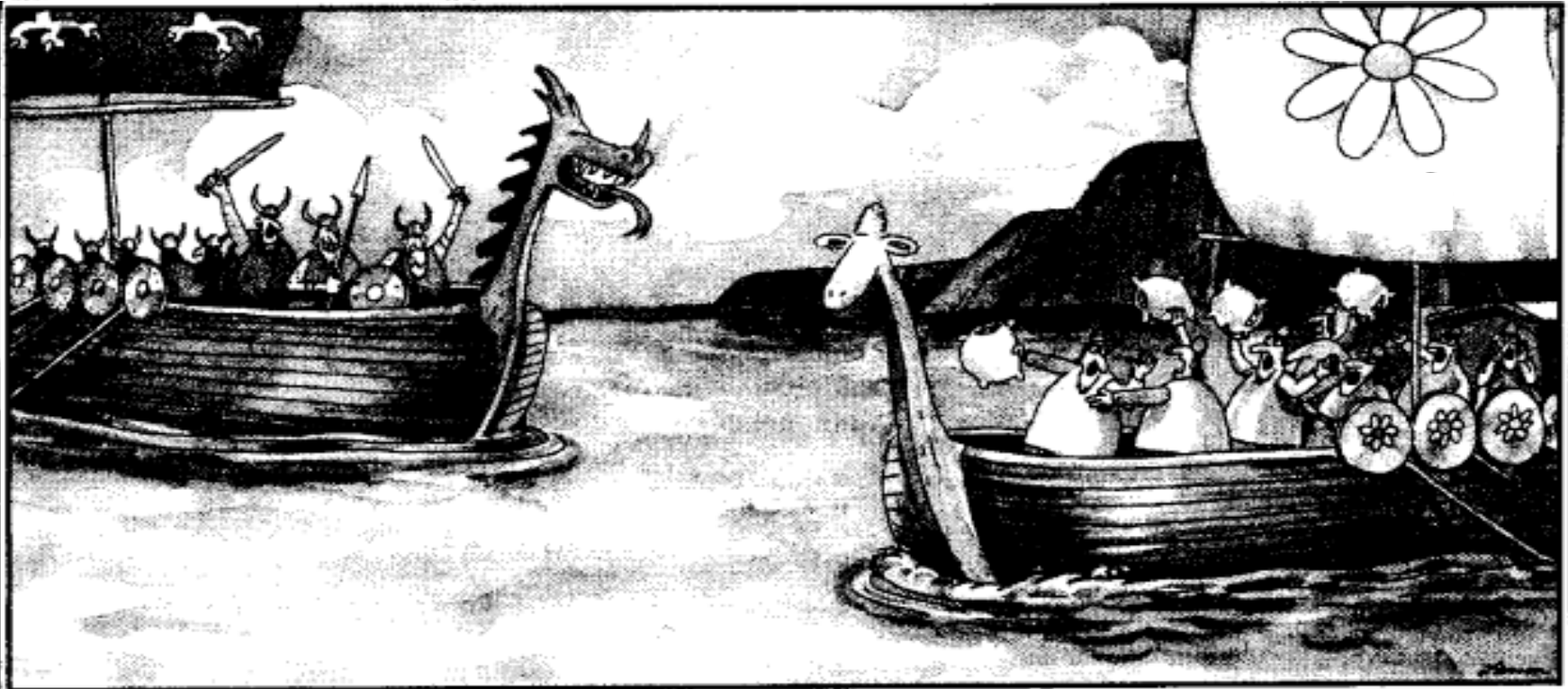
Recommendations to RPMs:

- Make sure non-specific methods data are confirmed
- When needed, review chromatograms/involve chemist
- Ask for Tentatively Identified Compounds Lists (90% hits)
- When the data doesn’t “look right” :



Data File: /chem/varian73,i/r010804d,b/042rFULL4TA,d
 Date : 05-MIG-2001 09:54
 Client ID: FULL4TA
 Sample Info: FULL4TA

It may not be right! Always double check data when needed. Be properly “armed” before making \$\$\$ decisions.



Although skilled with their pillow arsenal, the Wimpodites were favorite targets of Viking attacks.